AS ENCLOSED TO IPER

We claim:

1. A process for preparing 3-cyano-3,5,5-trimethylcyclohexanone (isophoronenitrile) by reacting isophorone with hydrogen cyanide in the presence of a base as a catalyst selected from alkali metal and alkaline earth metal cyanides, alkali metal and alkaline earth metal hydroxides, alkali metal and alkaline earth metal oxides and alkali metal and alkaline earth metal alcoholates to obtain a crude isophoronenitrile product, and subsequently distilling the crude isophoronenitrile product, which comprises adding, before a distillation, at least one sulfonic acid or carboxylic acid selected from the group consisting of

$$R\text{-}SO_3H$$

where R is a linear or branched C_1- to C_{24}-alkyl radical which may optionally be substituted by $-CO_2R'$ where R' is hydrogen or an alkyl radical, or by a phosphonic acid group, a phenyl radical substituted by linear or branched C_2- to C_{24}-alkyl radicals, nitro, sulfo or hydroxyl groups; or a substituted or unsubstituted fused aromatic radical; aliphatic polysulfonic acids; condensates of naphthalene- or phenolsulfonic acids, aliphatic polycarboxylic acids; and

$$R''\text{-}CO_2H$$

where R" is a linear or branched C_2- to C_{24}-alkyl radical which may optionally be substituted by one or more phosphonic acid groups; a phenyl radical which is unsubstituted or substituted by linear or branched C_1- to C_{24}-alkyl groups, nitro, sulfo or hydroxyl groups; or an unsubstituted or substituted fused aromatic radical.

2. A process as claimed in claim 1, wherein the carboxylic acid or sulfonic acid is added in an amount of 1 acid equivalent, based on 1 base equivalent of the base used as the catalyst.

3. A process as claimed in claim 1 or 2, wherein the base used as the catalyst is used in an amount of from 0.01 to 20% by weight, based on the isophorone used.

4. A process as claimed in any of claims 1 to 3, wherein the reaction is carried out at temperatures of from 80 to 220°C, preferably from 120 to 200°C, more preferably from 150 to 200°C.

5. A process as claimed in any of claims 1 to 4, wherein the reaction is carried out at a pressure of from 1 to 5 bar, preferably from 1 to 3 bar.

6. A process as claimed in any of claims 1 to 5, wherein the distillation is carried out in a rectification column.

7. A process as claimed in any of claims 1 to 6, wherein the reaction, the addition of the sulfonic acid or carboxylic acid and the subsequent distillation are carried out continuously.

8. A process as claimed in any of claims 1 to 7, wherein at least one acid selected from the group consisting of naphthalenesulfonic acids, alkyl-substituted naphthalenesulfonic acids and alkyl-substituted benzenesulfonic acids having an alkyl radical having ≥ 4 carbon atoms is used before the distillation.

9. A process for preparing 3-cyano-3,5,5-trimethylcyclohexanes (isophoronenitrile) comprising the following steps:

a) isophoronenitrile synthesis by reaction of isophorone with hydrogen cyanide in the presence of a base as a catalyst selected from alkali metal and alkaline earth metal cyanides, alkali metal and alkaline earth metal hydroxides, alkali metal and alkaline earth metal oxides and alkali metal and alkaline earth metal alcoholates to obtain a crude isophoronenitrile product,

b) neutralization of the reaction mixture obtained in step a) with a sulfonic acid or carboxylic acid selected from the group consisting of

$$R\text{-}SO_3H$$

where R is a linear or branched C_1- to C_{24}-alkyl radical which may optionally be substituted by $-CO_2R'$ where R' is hydrogen or an alkyl radical, or by one or more phosphonic acid groups, a phenyl radical substituted by linear or branched C_2- to C_{24}-alkyl radicals, nitro, sulfo or hydroxyl groups; or a substituted or unsubstituted fused aromatic radical; aliphatic polysulfonic

acids; condensates of naphthalene- or phenolsulfonic acids, aliphatic polycarboxylic acids; and

$$R''\text{-}CO_2H$$

where R" is a linear or branched C_2- to C_{24}-alkyl radical which may optionally be substituted by one or more phosphonic acid groups; a phenyl radical which is substituted by linear or branched C_1- to C_{24}-alkyl groups, nitro, sulfo or hydroxyl groups; or an unsubstituted or substituted fused aromatic radical,

c) distillation of the reaction mixture obtained in step b).

10. A process as claimed in claim 9, wherein the neutralization in step b) is carried out with a sulfonic acid selected from the group consisting of naphthalenesulfonic acids, alkyl-substituted naphthalenesulfonic acids and alkyl-substituted benzenesulfonic acids having an alkyl radical having ≥ 4 carbon atoms.

11. The use of a sulfonic acid or carboxylic acid as claimed in claim 1 as a neutralizing agent before the distillation of a crude isophoronenitrile product which has been obtained by reacting isophorone with hydrogen cyanide in the presence of a base selected from alkali metal and alkaline earth metal cyanides, alkali metal and alkaline earth metal hydroxides, alkali metal and alkaline earth metal oxides and alkali metal and alkaline earth metal alcohloates as a catalyst, in order to avoid precipitates in the neutralization of the base used as the catalyst with an acid.

12. The use as claimed in claim 11, wherein a sulfonic acid is used selected from the group consisting of naphthalenesulfonic acids, alkyl-substituted naphthalene sulfonic acids and alkyl-substituted benzenesulfonic acids having an alkyl radical having ≥ 4 carbon atoms.

13. A process for preparing 3-cyano-3,5,5-trimethylcyclohexanone (isophoronenitrile) by reacting isophorone with hydrogen cyanide in the presence of a base as a catalyst selected from alkali metal and alkaline earth metal cyanides, alkali metal and alkaline earth metal hydroxides, alkali metal and alkaline earth metal oxides and alkali metal and alkaline earth metal alcoholates to obtain a crude isophoronenitrile product, and subsequently distilling the crude isophoronenitrile product, which comprises adding, before a distillation, at least one sulfonic acid or carboxylic acid selected from the group consisting of naphthalenesulfonic acids,

alkyl-substituted naphthalenesulfonic acids and alkyl-substituted benzenesulfonic acids having an alkyl radical having ≥ 4 carbon atoms.

14. A process for preparing 3-cyano-3,5,5-trimethylcyclohexanes (isophoronenitrile) as claimed in claim 13 comprising the following steps:

a) isophoronenitrile synthesis by reaction of isophorone with hydrogen cyanide in the presence of a base as a catalyst selected from alkali metal and alkaline earth metal cyanides, alkali metal and alkaline earth metal hydroxides, alkali metal and alkaline earth metal oxides and alkali metal and alkaline earth metal alcoholates to obtain a crude isophoronenitrile product,

b) neutralization of the reaction mixture obtained in step a) with a sulfonic acid selected from the group consisting of naphthalenesulfonic acids, alkyl-substituted naphthalenesulfonic acids and alkyl-substitutes benzenesulfonic acids having an alkyl radical having ≥ 4 carbon atoms,

15. The use of a sulfonic acid selected from the group consisting of naphtahlenesulfonic acids, alkyl-substituted naphthalenesulfonic acids and alkyl-substituted benzenesulfonic acids having an alkyl radical having ≥ 4 carbon atoms as a neutralizing agent before the distillation of a crude isophoronenitrile product which has been obtained by reacting isophorone with hydrogen cyanide in the presence of a base selected from alkali metal and alkaline earth metal cyanides, alkali metal and alkaline earth metal hydroxides, alkali metal and alkaline earth metal oxides and alkali metal and alkaline earth metal alcohloates as a catalyst, in order to avoid precipitates in the neutralization of the base used as the catalyst with an acid.

16. A process as claimed in claim 13 or 14, wherein the sulfonic acid is diisobutylnaphthalenesulfonic acid or dodecylbenzenesulfonic acid.

17. The use as claimed in claim 15, wherein the sulfonic acid is diisobutylnaphthalenesulfonic acid or dodecylbenzenesulfonic acid.

18. A process as claimed in any of claims 1 to 7, wherein the base is sodium cyanide and the at least one sulfonic acid or carboxylic acid is selected from the group consisting of toluenesulfonic acid, mthanesulfonic acid, diisobutylnaphthalenesulfonic acid, dodecylbenzenesulfonic acid and 2-ethylhexanoic acid.

19. The use as claimed in claim 11, wherein the sulfonic acid or carboxylic acid is selected from the group consisting of toluenesulfonic acid, methanesulfonic acid, diisobutylnaphthalenesulfonic acid, dodecylbenzenesulfonic acid and 2-ethylhexanoicacid, and the base is sodium cyanide.